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Triplet oxygen-water associates as the main agents of acidifying autocatalytic redox-processes. Quantum-chemical description of primary elementary acts of combustion

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Abstract

The potential reaction systems involving triplet oxygen-water associates, alkanes, alkenes, and hydrogen using the Woodward-Hoffmann rule are described. A new quantum-chemical interpretation of primary acts of combustion are presented.

For the first time it was demonstrated, that the act of interaction of molecular triplet oxygen $^3O_2$ with various proton-donating agents is carried out with the participation of a water associate by a radical mechanism, which means the presence of an autocatalytic process catalyzed by water molecule.

The triplet water-oxygen associate is also attached by a radical aqueous O-H group to sp^2 hybridized ethylene carbon to form a hydroperoxide and hydroxyethyl radicals.

The participation of water in the form of an associative agent removes orbital symmetry prohibition for triplet oxygen, but the effect of reducing the activation indices is so significant that this requires additional research to remove this problem. The solution of the problem can be either the registration of specific solvation by large clusters of water, the presence of third reagents or impacts, or more accurate calculations using Time-dependent density functional theory (TDDFT).

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